

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
 Data File : BG048862.D
 Acq On : 23 Apr 2021 14:10
 Operator : CG/JU
 Sample : M2107-10
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-31-10.5-11.0

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048862.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.124	298	304	308	rBV2	13569	21412	1.87%	0.255%
2	5.606	379	386	393	rBV	402165	622143	54.40%	7.399%
3	7.222	650	661	673	rVB	404084	727861	63.64%	8.656%
4	8.050	791	802	809	rBV	100408	173942	15.21%	2.069%
5	8.185	818	825	830	rBV	43740	69744	6.10%	0.829%
6	8.267	835	839	846	rVB6	11001	17225	1.51%	0.205%
7	8.831	930	935	940	rBV4	6901	12538	1.10%	0.149%
8	9.225	995	1002	1010	rBV	274130	473440	41.40%	5.631%
9	10.876	1278	1283	1289	rBV	123347	215625	18.85%	2.564%
10	12.274	1515	1521	1527	rBV6	6624	13737	1.20%	0.163%
11	13.332	1694	1701	1710	rVB	617100	942534	82.41%	11.209%
12	13.520	1729	1733	1739	rVB5	7462	12826	1.12%	0.153%
13	13.585	1739	1744	1748	rBV5	9700	16502	1.44%	0.196%
14	13.920	1795	1801	1807	rVB4	8025	13315	1.16%	0.158%
15	14.155	1835	1841	1849	rVB	22778	50540	4.42%	0.601%
16	14.595	1912	1916	1919	rBV4	8400	12081	1.06%	0.144%
17	14.713	1930	1936	1944	rVB2	199880	311370	27.23%	3.703%
18	15.195	2013	2018	2022	rBV6	8323	13117	1.15%	0.156%
19	15.277	2027	2032	2037	rVB7	21875	34203	2.99%	0.407%
20	15.500	2065	2070	2073	rBV5	8181	16190	1.42%	0.193%
21	16.205	2184	2190	2202	rBV	493762	775950	67.85%	9.228%
22	16.428	2221	2228	2234	rBV7	20587	39087	3.42%	0.465%
23	17.468	2400	2405	2410	rBV	230508	356559	31.18%	4.240%
24	19.848	2807	2810	2813	rBV4	43869	55672	4.87%	0.662%
25	20.083	2846	2850	2856	rVB	927580	1143688	100.00%	13.602%
26	20.300	2884	2887	2891	rVB	73729	83232	7.28%	0.990%
27	21.387	3068	3072	3079	rVB	104330	144845	12.66%	1.723%
28	21.575	3100	3104	3109	rVB5	70368	105203	9.20%	1.251%
29	21.646	3112	3116	3120	rVB2	136918	196109	17.15%	2.332%
30	21.710	3123	3127	3130	rBV6	53800	79501	6.95%	0.945%
31	21.769	3132	3137	3142	rVB	209436	365808	31.98%	4.350%
32	22.574	3271	3274	3277	rVB4	44160	56239	4.92%	0.669%
33	22.639	3279	3285	3291	rVB	347786	608398	53.20%	7.236%
34	22.827	3315	3317	3335	rVB	82755	218652	19.12%	2.600%
35	25.101	3696	3704	3713	rVB2	136520	391129	34.20%	4.652%
36	31.675	4820	4823	4826	rBV5	10296	18051	1.58%	0.215%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

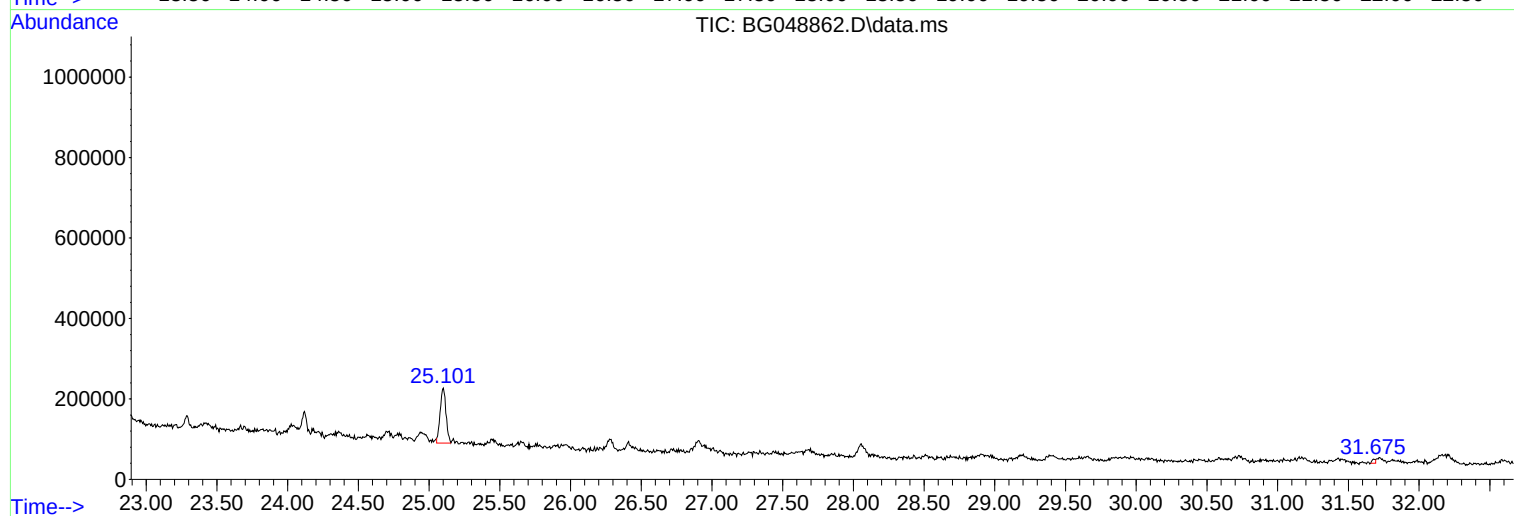
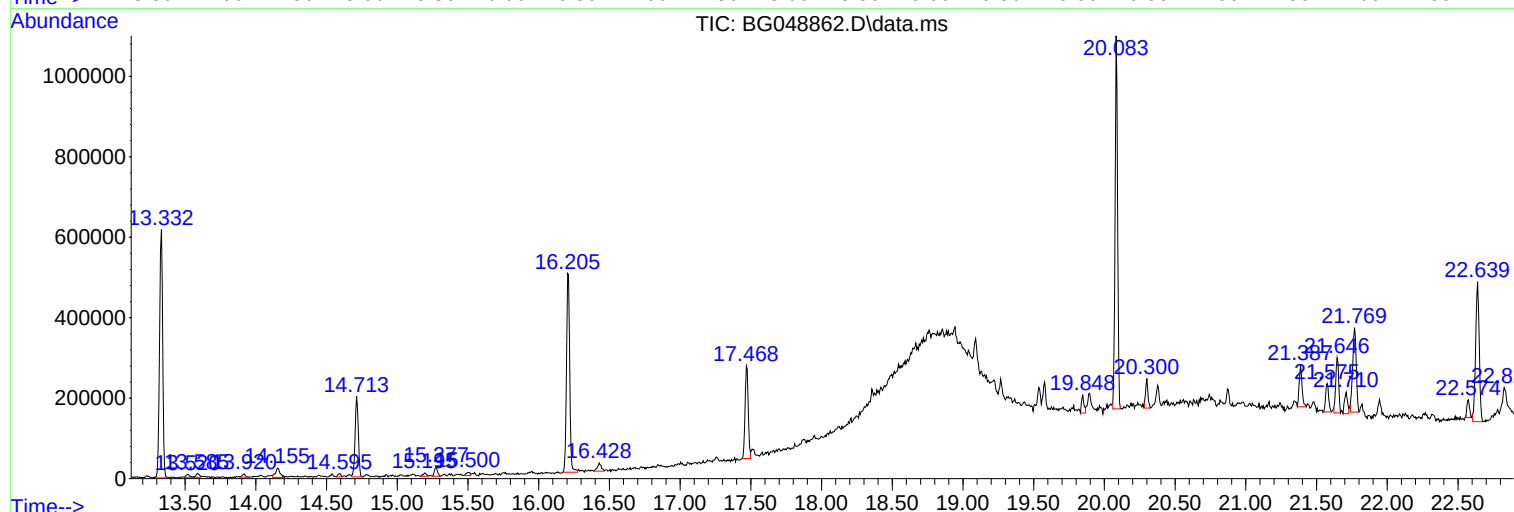
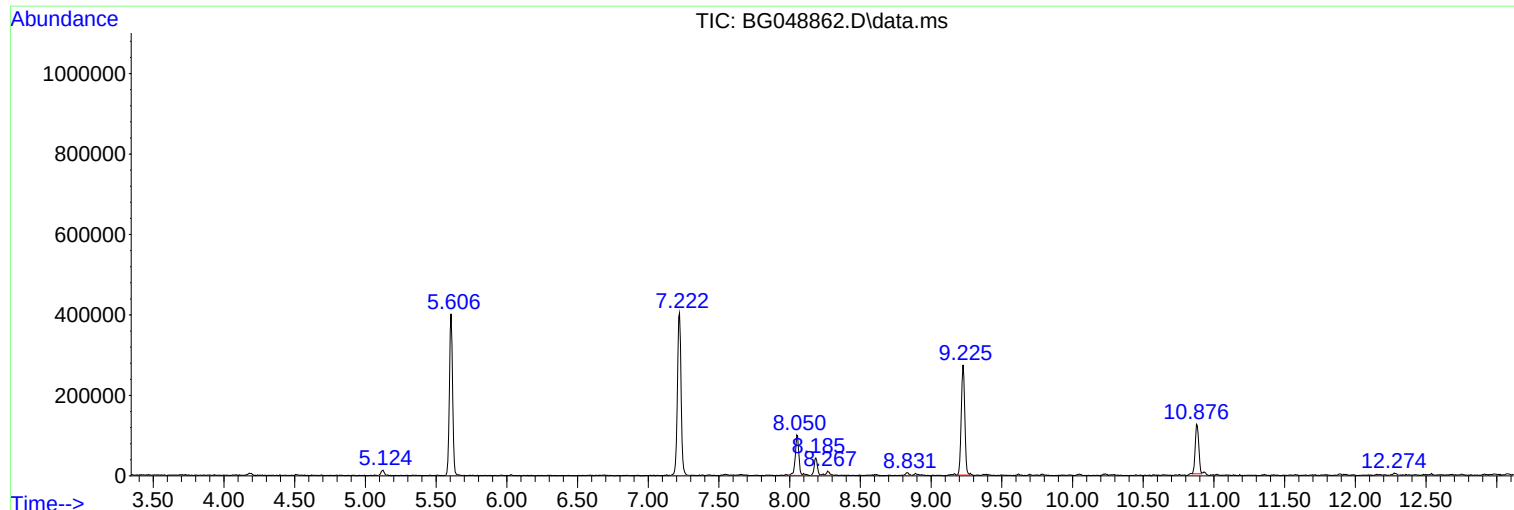
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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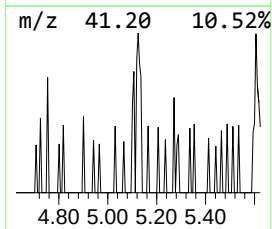
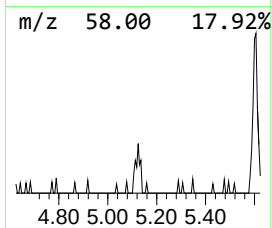
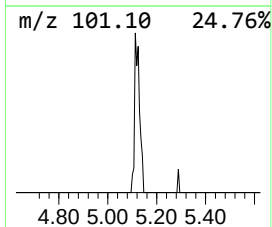
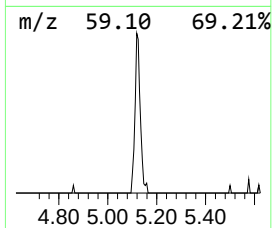
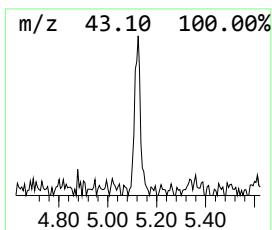
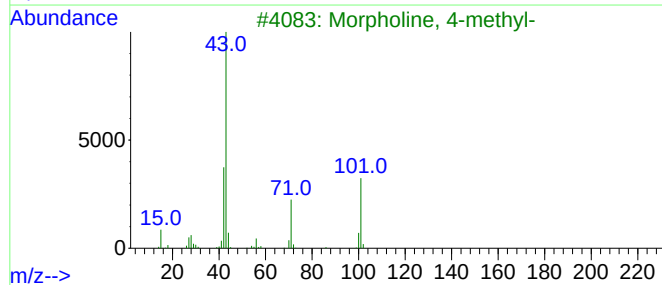
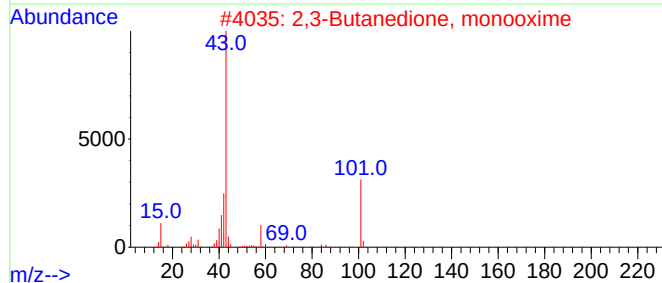
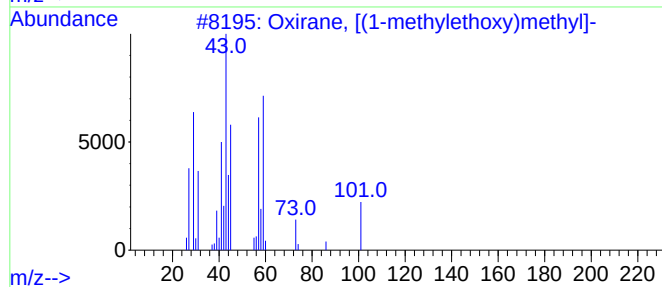
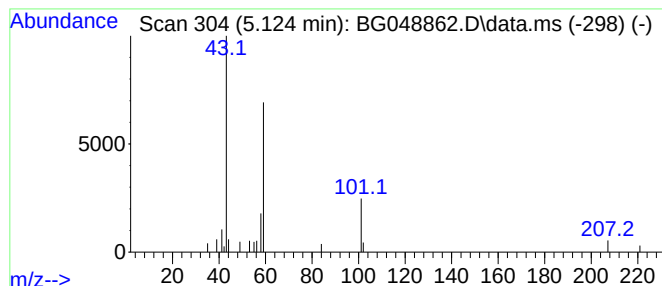
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown5.12 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.124	2.46 ng	21412	1,4-Dichlorobenzene-d4	8.056

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	38		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9		
5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9		



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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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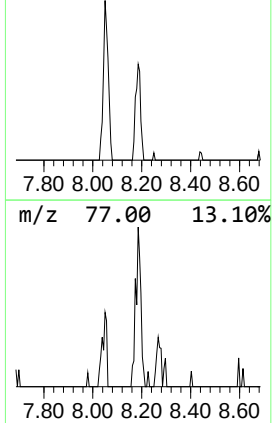
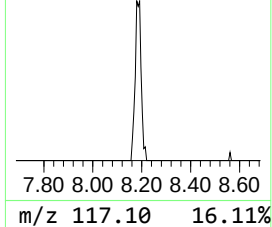
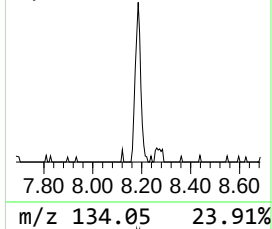
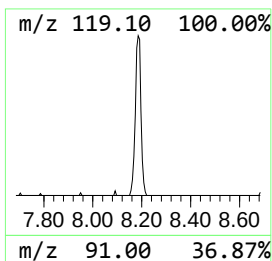
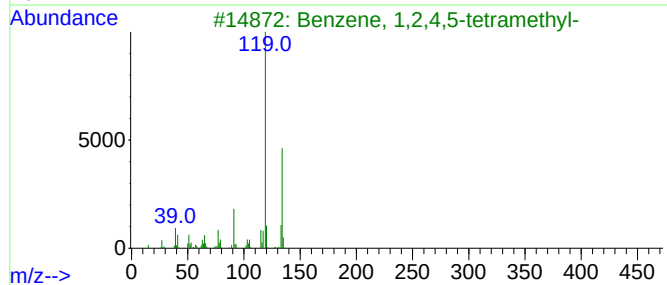
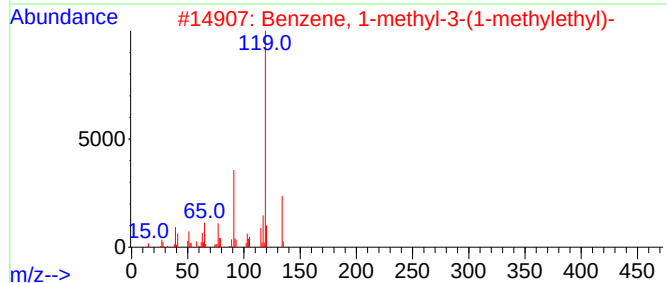
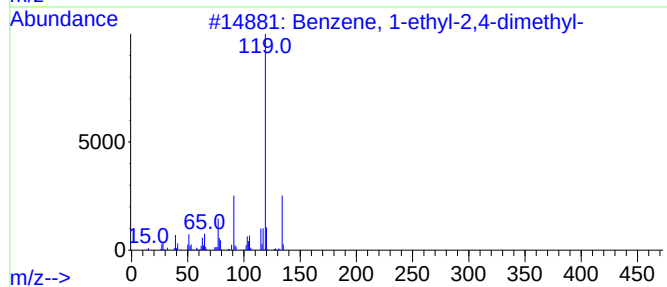
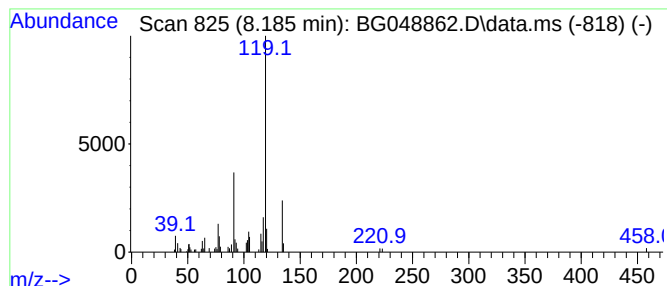
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.185	8.02 ng	69744	1,4-Dichlorobenzene-d4	8.056

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	91
2			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	90
3			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	90
4			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	90
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	87



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BNA_G
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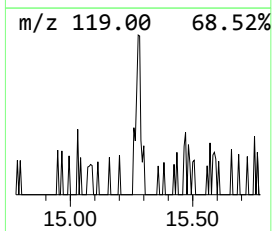
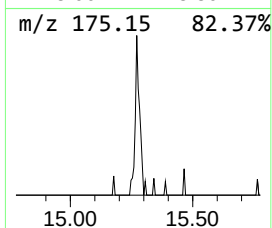
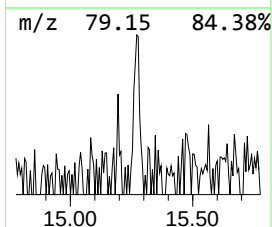
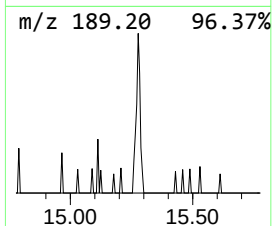
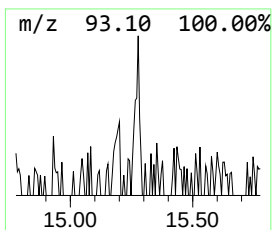
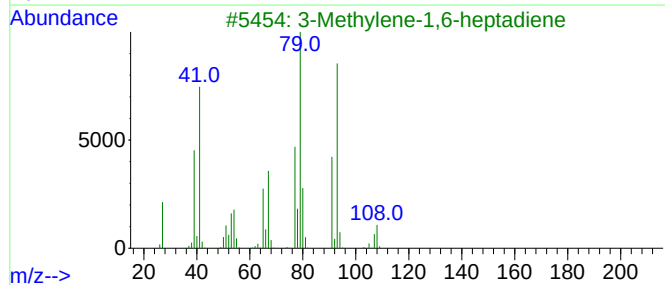
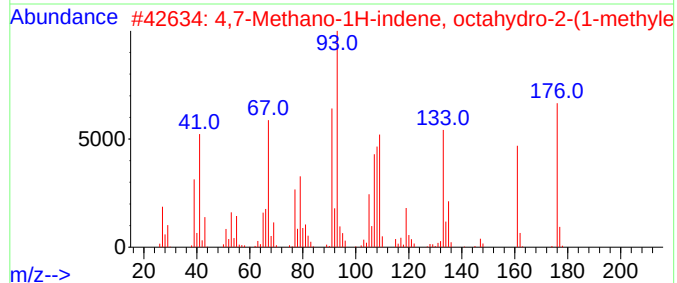
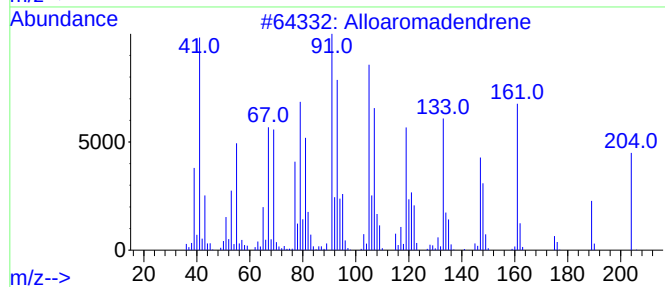
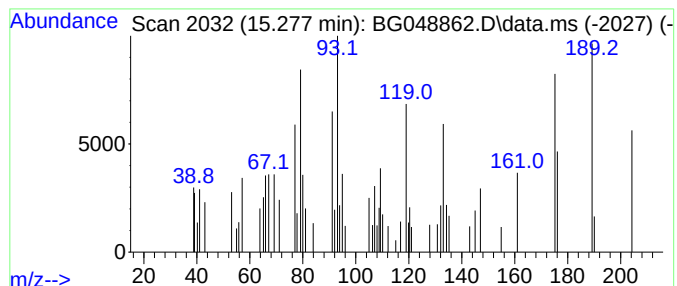
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown15.22 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.277	2.20 ng	34203	Acenaphthene-d10	14.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Alloaromadendrene	204	C15H24	025246-27-9	38
2			4,7-Methano-1H-indene, octahydro...	176	C13H20	074793-54-7	30
3			3-Methylene-1,6-heptadiene	108	C8H12	016626-48-5	25
4			Bicyclo[3.1.1]hept-2-ene, 2,6-di...	204	C15H24	017699-05-7	22
5			cis-(-)-2,4a,5,6,9a-Hexahydro-3,...	204	C15H24	1000104-20-1	20



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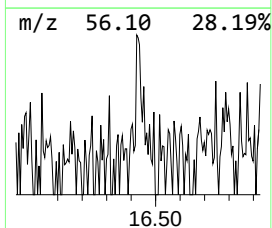
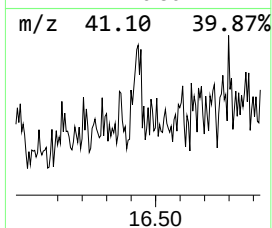
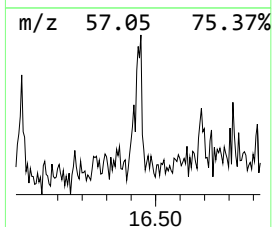
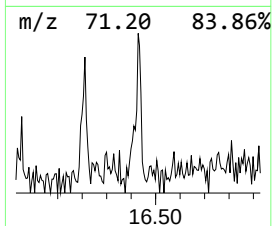
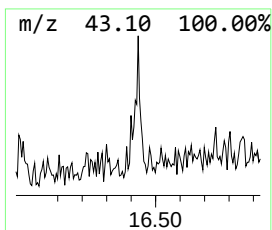
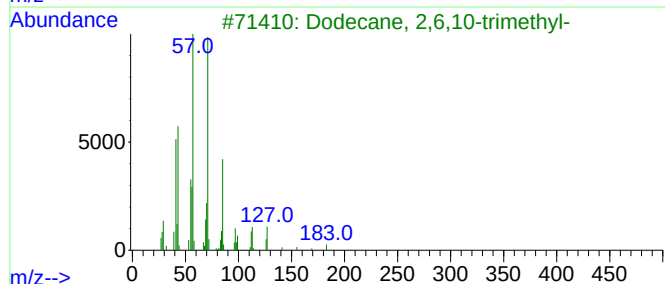
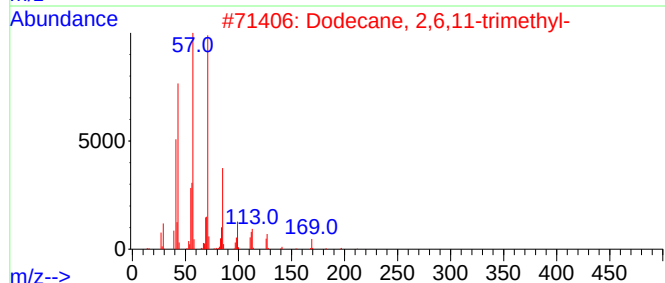
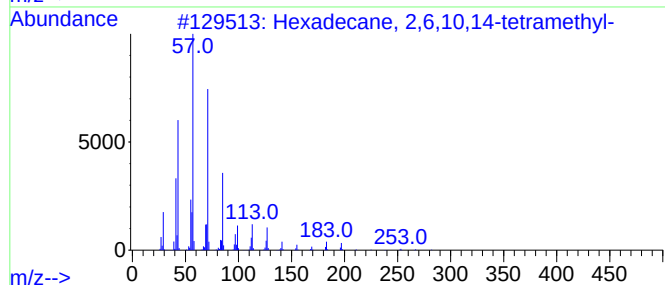
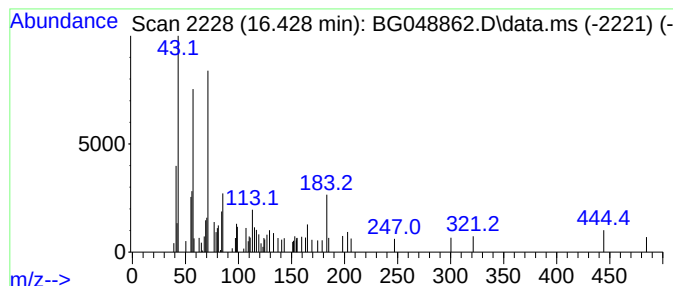
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane, 2,6,10,14-tetra... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.428	2.19 ng	39087	Phenanthrene-d10		17.468	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-		282	C20H42	000638-36-8	50
2	Dodecane, 2,6,11-trimethyl-		212	C15H32	031295-56-4	47
3	Dodecane, 2,6,10-trimethyl-		212	C15H32	003891-98-3	47
4	Hexadecane, 2,6,11,15-tetramethyl-		282	C20H42	000504-44-9	47
5	Octane, 1-iodo-		240	C8H17I	000629-27-6	43



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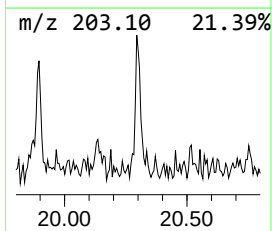
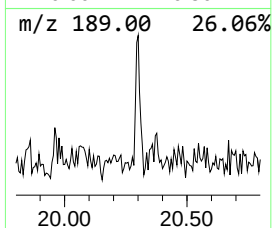
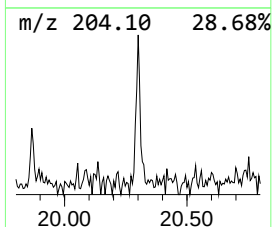
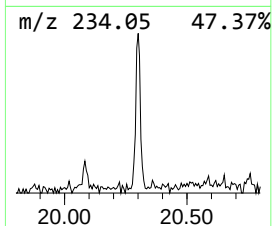
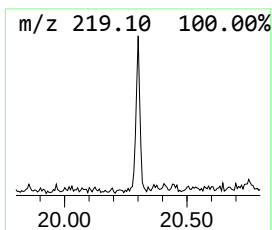
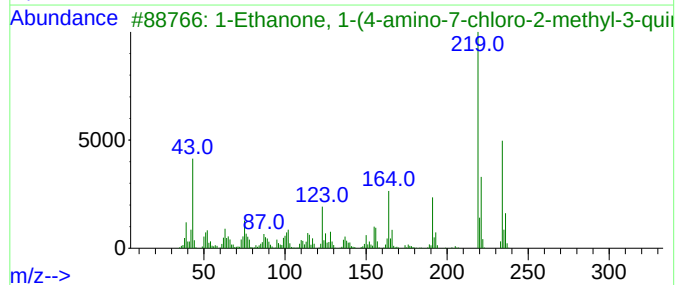
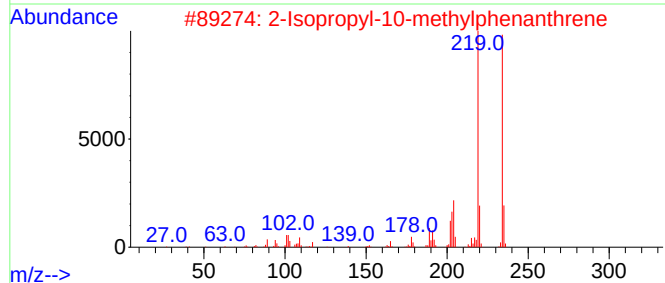
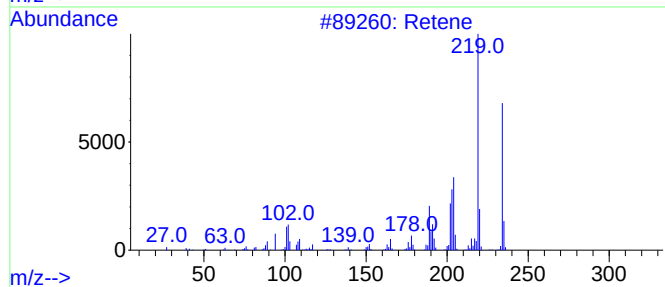
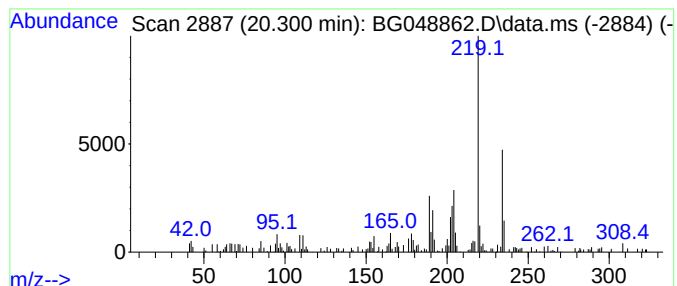
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Retene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.300	4.55 ng	83232	Chrysene-d12	21.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Retene	234	C18H18	000483-65-8	83
2			2-Isopropyl-10-methylphenanthrene	234	C18H18	066552-97-4	81
3			1-Ethanone, 1-(4-amino-7-chloro-...	234	C12H11ClN2O	1000350-06-0	53
4			3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	50
5			2,3,5,6-Detetrahydrocyclohexanon...	234	C15H22O2	101100-38-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048862.D
Acq On : 23 Apr 2021 14:10
Operator : CG/JU
Sample : M2107-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-31-10.5-11.0

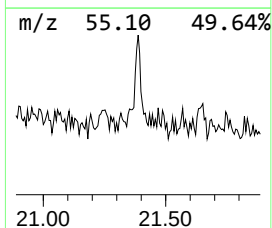
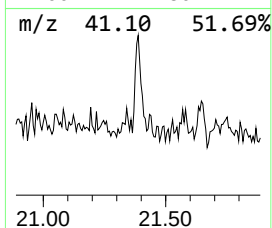
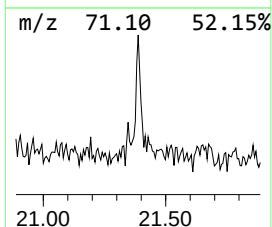
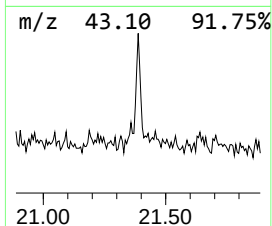
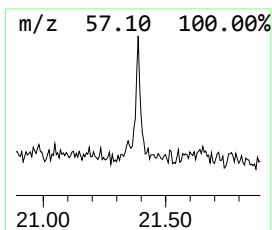
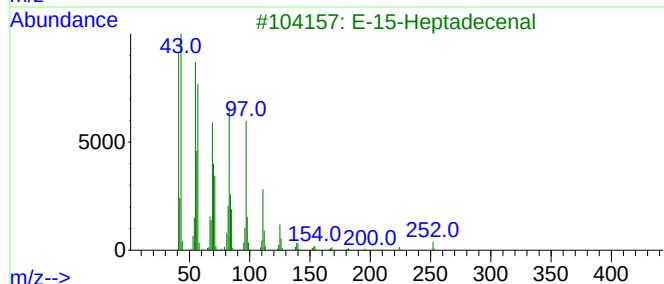
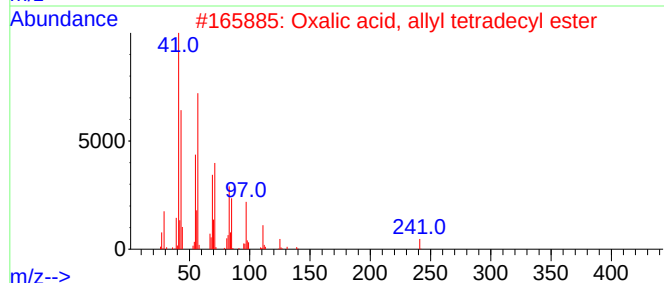
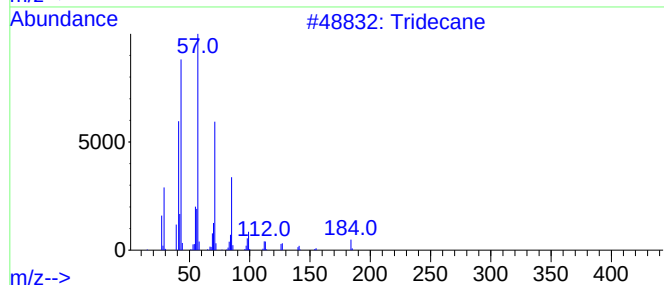
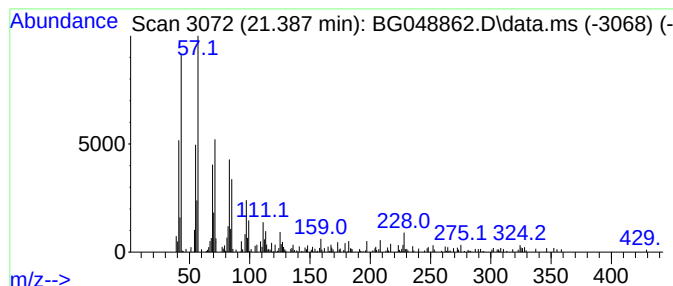
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.387	7.92 ng	144845	Chrysene-d12	21.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	80
2			Oxalic acid, allyl tetradecyl ester	326	C19H34O4	1000309-24-2	74
3			E-15-Heptadecenal	252	C17H32O	1000130-97-9	56
4			Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	55
5			1-Docosene	308	C22H44	001599-67-3	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048862.D
Acq On : 23 Apr 2021 14:10
Operator : CG/JU
Sample : M2107-10
Misc :
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Instrument :
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ClientSampleId :
SB-31-10.5-11.0

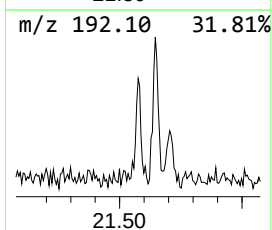
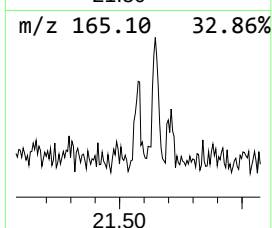
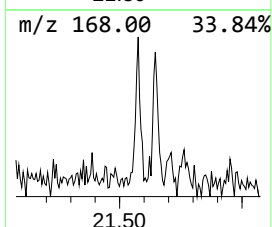
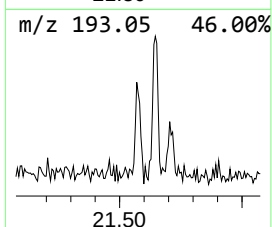
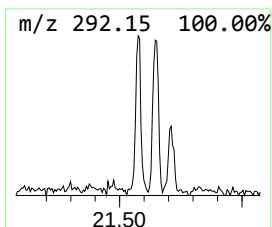
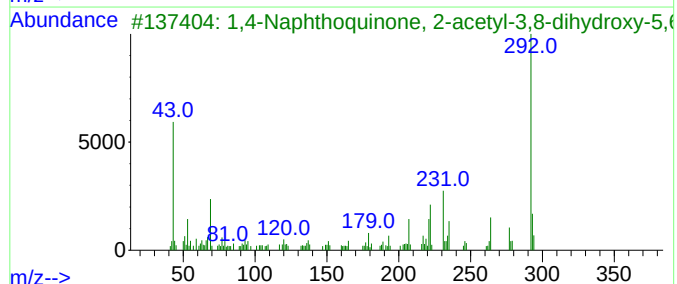
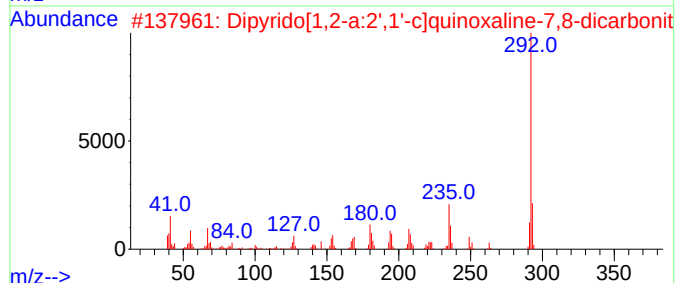
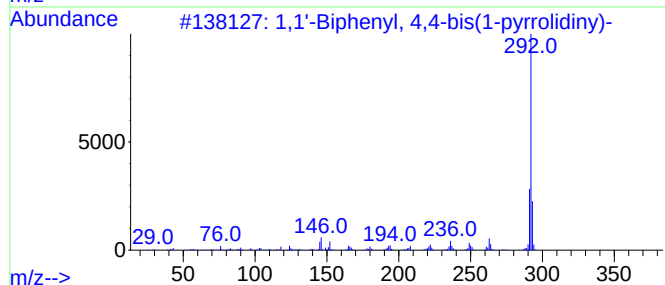
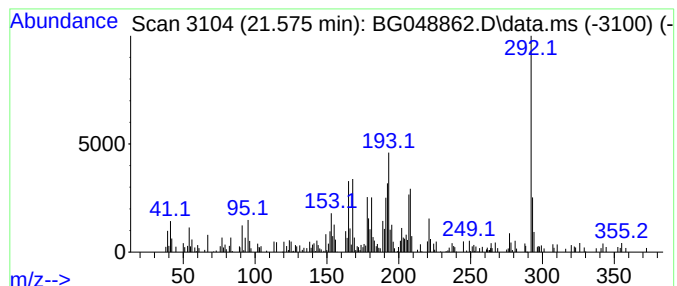
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown21.57 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.575	5.75 ng	105203	Chrysene-d12	21.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 4,4-bis(1-pyrroli...	292	C20H24N2	1000193-54-6	38		
2	Dipyrido[1,2-a:2',1'-c]quinoxali...	292	C18H20N4	1000303-96-3	38		
3	1,4-Naphthoquinone, 2-acetyl-3,8...	292	C14H12O7	014090-53-0	32		
4	4H,6H-1,3,5-Triazino[2,1-b]1,3,4...	292	C11H9ClN6S	311331-61-0	30		
5	Benzoic acid, 4-[2-(2-hydroxy-1-...	292	C17H12N2O3	1000197-03-1	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048862.D
Acq On : 23 Apr 2021 14:10
Operator : CG/JU
Sample : M2107-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-31-10.5-11.0

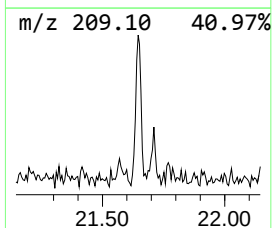
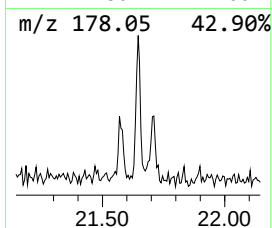
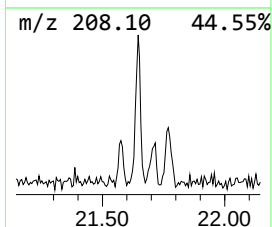
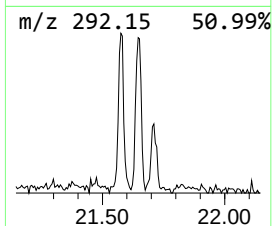
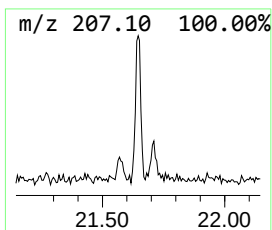
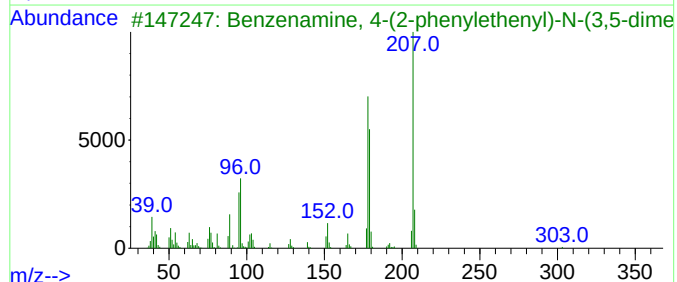
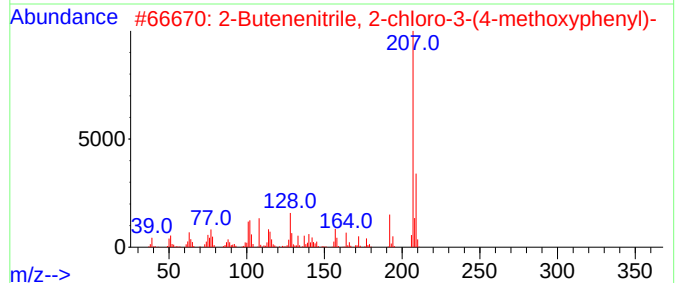
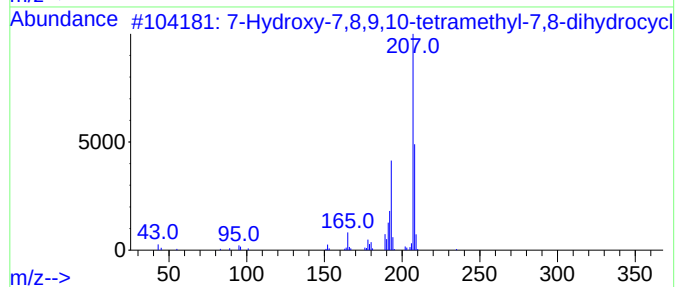
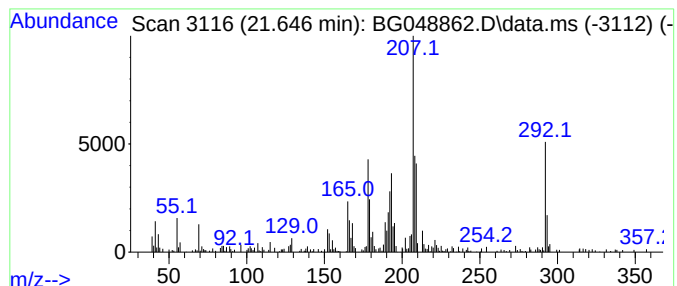
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown21.64 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.646	10.72 ng	196109	Chrysene-d12	21.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hydroxy-7,8,9,10-tetramethyl-7...	252	C18H20O	1000110-34-9	38		
2	2-Butenenitrile, 2-chloro-3-(4-m...	207	C11H10ClNO	1000305-66-7	35		
3	Benzenamine, 4-(2-phenylethenyl)...	303	C20H21N3	1000260-49-5	35		
4	2-Chloroaniline-5-sulfonic acid	207	C6H6ClNO3S	000098-36-2	27		
5	2-(Acetoxymethyl)-3-(methoxycarb...	282	C17H14O4	093103-70-9	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048862.D
Acq On : 23 Apr 2021 14:10
Operator : CG/JU
Sample : M2107-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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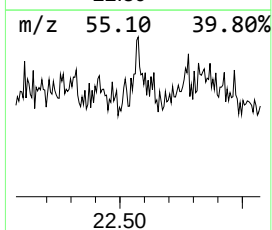
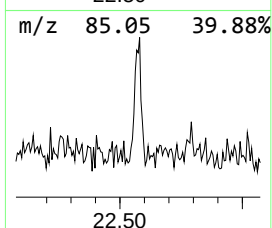
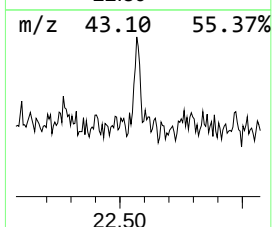
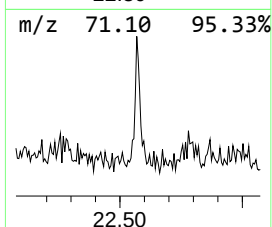
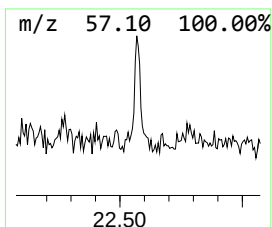
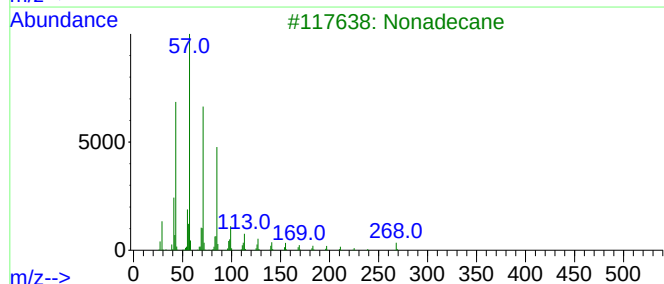
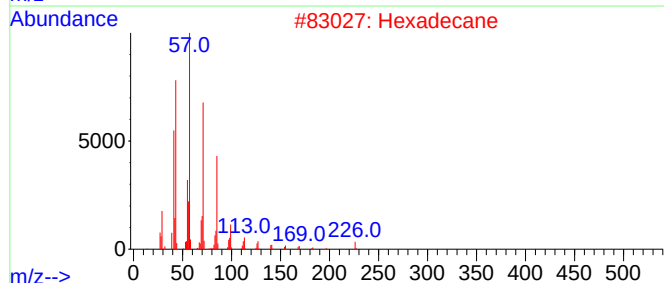
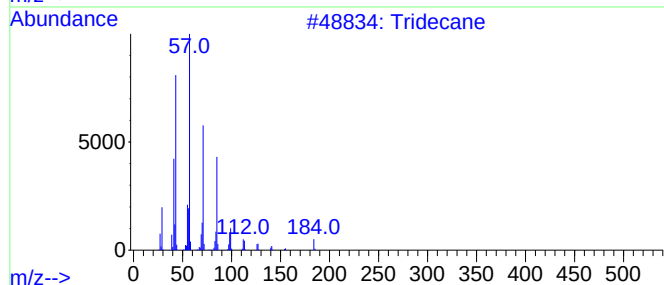
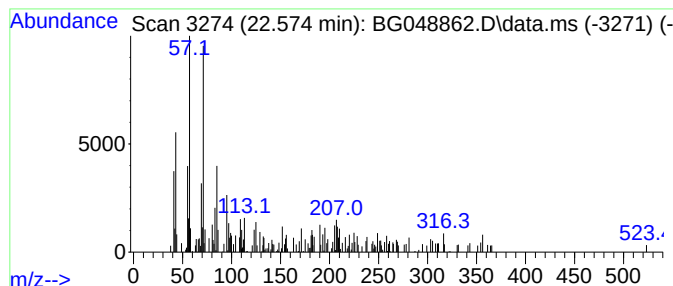
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown22.57 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.574	3.07 ng	56239	Chrysene-d12	21.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	55
2			Hexadecane	226	C16H34	000544-76-3	42
3			Nonadecane	268	C19H40	000629-92-5	42
4			Tetradecane	198	C14H30	000629-59-4	42
5			Docosane	310	C22H46	000629-97-0	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048862.D
Acq On : 23 Apr 2021 14:10
Operator : CG/JU
Sample : M2107-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-31-10.5-11.0

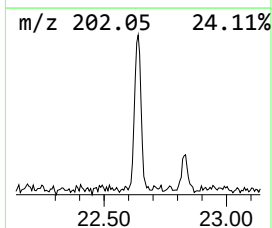
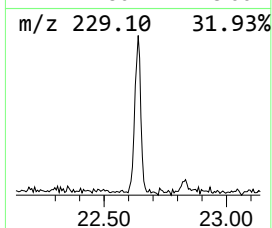
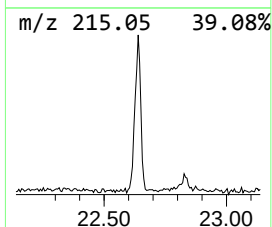
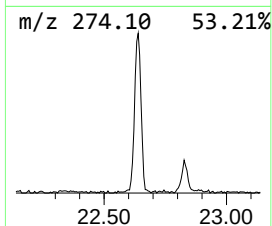
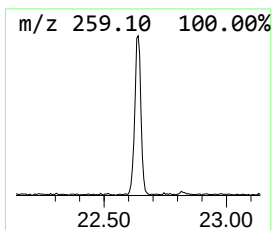
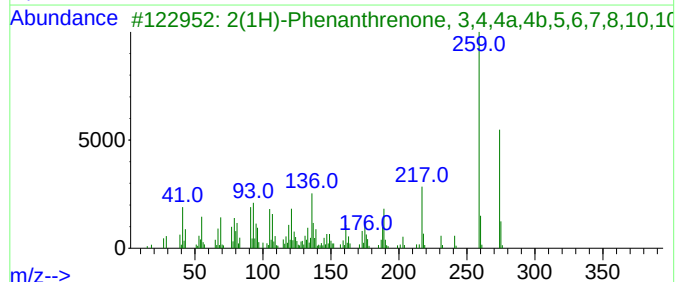
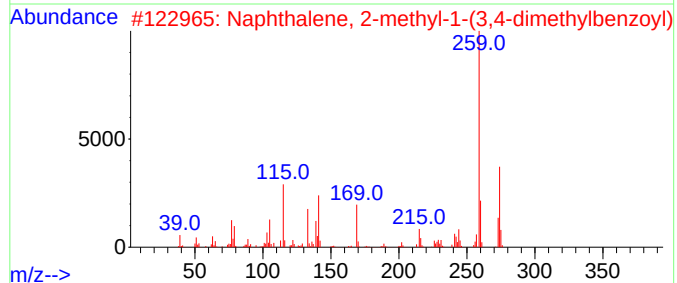
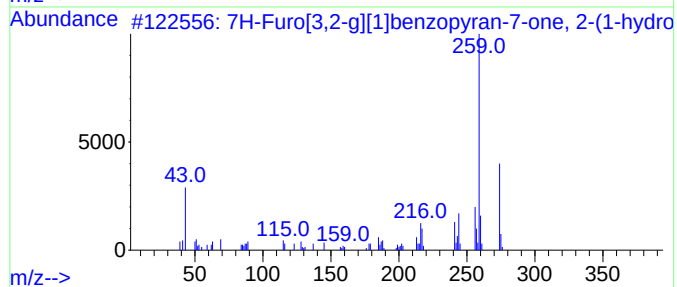
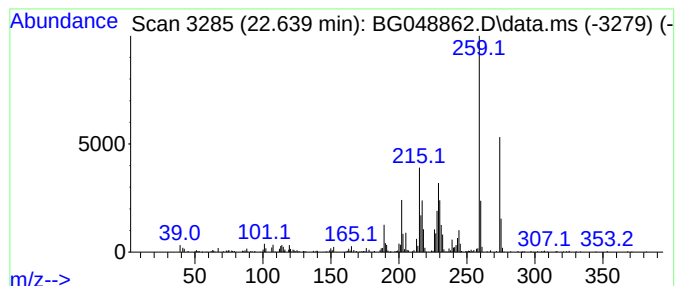
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 7H-Furo[3,2-g][1]benzopyran... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.639	33.26 ng	608398	Chrysene-d12	21.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7H-Furo[3,2-g][1]benzopyran-7-on...	274	C15H14O5	054087-32-0	50
2			Naphthalene, 2-methyl-1-(3,4-dim...	274	C20H18O	1000269-03-0	49
3			2(1H)-Phenanthrene, 3,4,4a,4b,...	274	C19H14O	007715-44-8	46
4			Propanamide, N-(1-ethyl-1,2,3,4-...	274	C17H26N2O	063134-09-8	43
5			9-Methyl-3-phenyl-9H-pyridazino(...	259	C17H13N3	003980-90-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048862.D
Acq On : 23 Apr 2021 14:10
Operator : CG/JU
Sample : M2107-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

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ClientSampleId :
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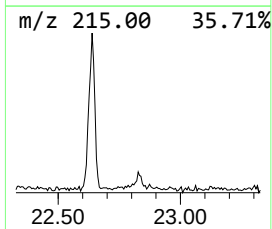
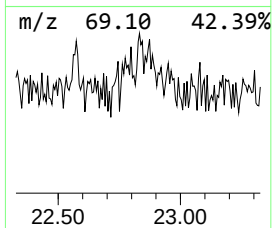
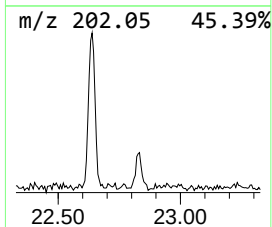
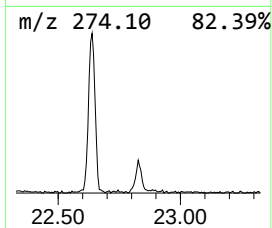
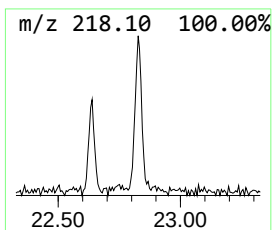
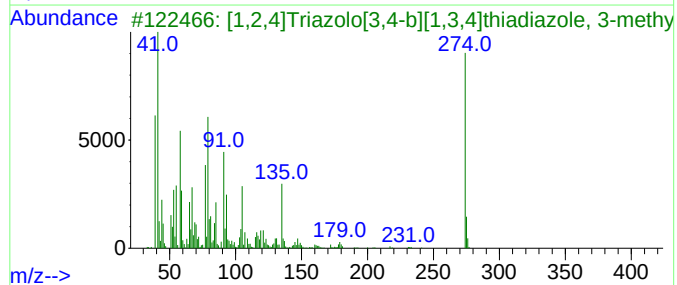
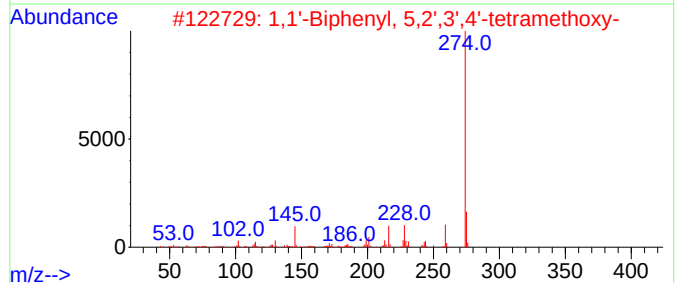
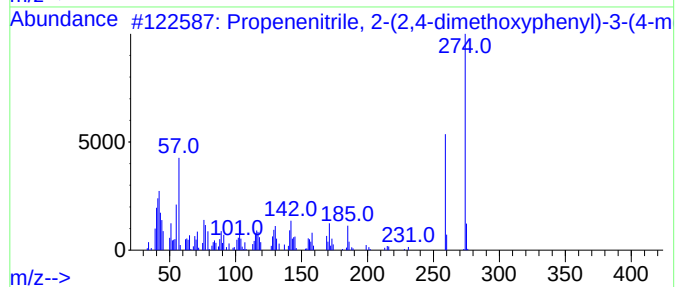
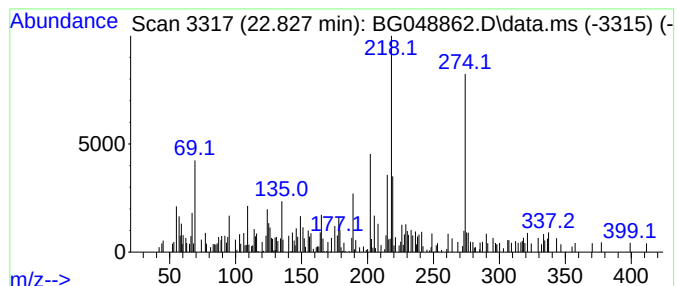
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown22.82 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.827	11.95 ng	218652	Chrysene-d12	21.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propenenitrile, 2-(2,4-dimethoxy...	274	C15H18N2O3	1000263-72-9	25
2			1,1'-Biphenyl, 5,2',3',4'-tetram...	274	C16H18O4	119101-30-3	25
3			[1,2,4]Triazolo[3,4-b][1,3,4]thi...	274	C14H18N4S	1000351-25-3	22
4			Pyrimidine-2,4,6(1H,3H,5H)-trion...	274	C13H14N4O3	346612-07-5	22
5			3,4,5,5-Tetrakis(methoxycarbonyl...	333	C13H19N09	071167-60-7	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048862.D
Acq On : 23 Apr 2021 14:10
Operator : CG/JU
Sample : M2107-10
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-31-10.5-11.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzene, 1-ethy...	8.185	8.0	ng	69744	1	8.056	173942	20.0
unknown15.22	15.277	2.2	ng	34203	3	14.713	311370	20.0
Hexadecane, 2,6...	16.428	2.2	ng	39087	4	17.468	356559	20.0
Retene	20.300	4.5	ng	83232	5	21.769	365808	20.0
Tridecane	21.387	7.9	ng	144845	5	21.769	365808	20.0
unknown21.57	21.575	5.8	ng	105203	5	21.769	365808	20.0
unknown21.64	21.646	10.7	ng	196109	5	21.769	365808	20.0
unknown22.57	22.574	3.1	ng	56239	5	21.769	365808	20.0
7H-Furo[3,2-g][...	22.639	33.3	ng	608398	5	21.769	365808	20.0
unknown22.82	22.827	11.9	ng	218652	5	21.769	365808	20.0